The microcanonical temperature in the Wang-Landau sampling

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In this paper we present a brief comment on the behavior of the slope of the entropy in the ground state. We show that the inverse temperature of the ground state diverges only for an infinite system and therefore the acute angle that the slope displays at this temperature is related to finite size effects.

Wang-Landau sampling (WLS)[1, 2] is the most widespread technique among the entropic algorithms. It simulates efficiently the density of states in a given test model. The heuristic idea of the method is based on the fact that if one performs a random walk in energy space with a probability proportional to the reciprocal of the density of states, a flat histogram is generated for the energy distribution. Since the density of states produces huge numbers, instead of estimating $g(E)$, the simulation is performed for $S(E) \equiv \ln g(E)$, and a histogram $H(E)$ is accumulated during the simulations to control the frequency of visits to the energy levels. At the beginning of the simulation we set $S(E) = 0$ for all energy levels. The random walk in the energy space runs through all energy levels from E_{min} to E_{max} with a probability

$$p(E \to E') = \min(\exp[S(E) - S(E')], 1), \tag{1}$$

where E and E' are the energies of the current and the new possible configurations. For each given model one should define a Monte Carlo sweep (e.g. L^2 spin-flip trial for the 2D Ising model or N monomer moves for a homopolymer). After each Monte Carlo sweep we update $H(E') \to H(E') + 1$ and $S(E') \to S(E') + F$, where $F = \ln f$ (f is the so-called modification factor) [3]. The initial modification factor is taken as $f = f_0 = e = 2.71828...$. The flatness of the histogram is checked after a number of Monte Carlo (MC) steps and usually the histogram is considered flat if $H(E) > 0.8\langle H\rangle$, for all energies, where $\langle H\rangle$ is an average over the energies. If the flatness condition is fulfilled we update the modification factor to a finer one by setting $f_{i+1} = \sqrt{f_i}$ and reset the histogram $H(E) = 0$. Testing the behavior of the canonical averages during the simulations, one can determine the ideal modification factor to stop the simulations [3]. Having in hand the density of states, one can calculate the canonical average of any thermodynamic variable as

$$\langle X\rangle_T = \frac{\sum_E \langle X\rangle_E g(E) e^{-\beta E}}{\sum_E g(E) e^{-\beta E}}, \tag{2}$$

where $\langle X\rangle_E$ is the microcanonical average accumulated during the simulations and $\beta = 1/k_B T$, k_B is the Boltzmann constant and T is the temperature. One of the interesting features of the method is that it can also access some quantities, such as the free energy and entropy at any temperature, which are not directly available from conventional Monte Carlo simulations.

However, analyzing the simulation results in terms of the microcanonical ensemble, the logarithm of the density of states corresponds exactly to the definition of entropy

$$S = k_B \ln g(E). \tag{3}$$

The Boltzmann constant k_B ensures the agreement with the Kelvin scale of temperature, defined by

$$\frac{1}{T} = \frac{\partial S}{\partial E}. \tag{4}$$

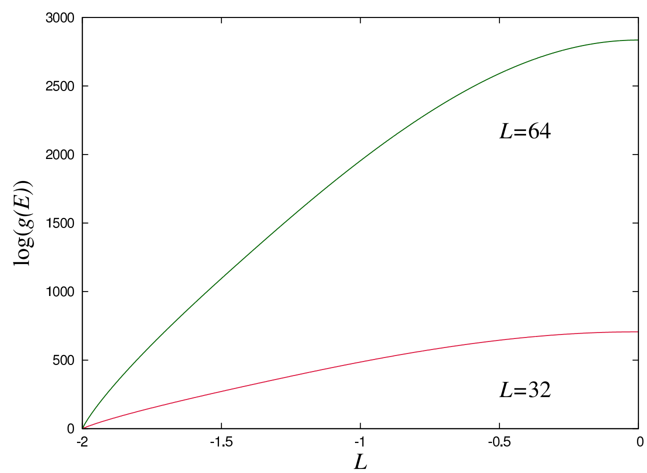

FIG. 1. Density of states obtained by Wang-Landau sampling for the 2D Ising model for $L = 32, 64$.

In this work we intend to shed some light on the reason why the slope of the density of states is not infinite in the ground state, where the inverse temperature diverges. In Fig. 1 we show the logarithm of the density of states of the 2D Ising model obtained by Wang-Landau sampling for two lattice sizes: $L = 32, 64$. One can see that indeed the slopes are not infinite in the ground state. Moreover, this behavior is also observed in the exact results of Beale[4]. The reason for this apparent contradiction are the finite-size effects. This situation resembles that of the magnetization in the Ising model, which for an infinite system drops to zero exactly at the critical temperature but presents a tail for finite sizes.

For any finite lattice in the 2D Ising model, the smallest ΔE from the ground state is given by

$$\Delta E = (E_{min} + 8) - E_{min} = 8. \tag{5}$$

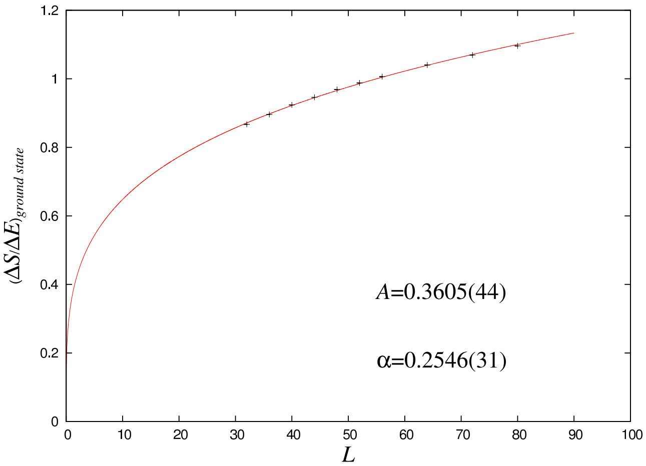

FIG. 2. Finite-size scaling behavior of $\frac{\Delta S}{\Delta E}$ as function of L.

Therefore, the limit in the derivative

$$\frac{\partial S}{\partial E} = \lim_{\Delta E \to 0} \frac{\Delta S}{\Delta E} \tag{6}$$

becomes exact only if $L \to \infty$ ($E_{min} = -2L^2 \to -\infty$).

In order to investigate the finite-size scaling behavior of the ratio $\Delta S/\Delta E$ we performed Wang-Landau simulations of the 2D Ising model with $L = 32, 36, 40, 44, 48, 52, 56, 64, 72$ and 80, taking $N = 24, 24, 20, 20, 20, 16, 16, 16, 12$ and 12 independent runs for each size, respectively.

Setting k_B equal to unit, $S(E) \equiv \log(g(E))$. In Fig.2 we show that the derivative in the ground state scales as

$$\frac{\partial S(L)}{\partial E} = A L^{\alpha}, \tag{7}$$

where $A = 0.3605(44)$ and $\alpha = 0.2546(31)$.

One can see that $\frac{\Delta S}{\Delta E}$ does actually tends to infinity as $L \to \infty$. The misunderstanding is therefore related to finite size effects.

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[4] P. D. Beale, Phys. Rev. Lett. **76**, 78 (1996).